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# Translating environmental xenobiotic fate models across scales

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## Abstract

The classical models developed for degradation and transport of xenobiotics have been derived with the assumption of homogeneous environments. Unfortunately, deterministic models function well in the laboratory under homogeneous conditions but such homogeneous conditions often do not prevail in the field. A possible solution is the incorporation of the statistical variation of soil parameters into deterministic process models. This demands the development of stochastic models of spatial variability. To this end, spatial soil parameter fields are conceived as the realisation of a random spatial process.

Extrapolation of local fine scale models to large heterogeneous fields is achieved by coupling deterministic process models with random spatial field models.

## Notation:

$q$	: volumetric water flux density [cm/d]
$Q$	: $Q(x,y,z,t)$ = source and sink term for water-transport [cm <sup>3</sup> /cm <sup>3</sup> /d]
$p$	: hydraulic potential
$\rho$	: bulk density [g/cm <sup>3</sup> ]
$\theta$	: water content [cm <sup>3</sup> /cm <sup>3</sup> ]
$\theta_r$	: residual water content [cm <sup>3</sup> /cm <sup>3</sup> ]
$\theta_s$	: saturated water content [cm <sup>3</sup> /cm <sup>3</sup> ]
$\Theta$	: normalized water content (cf. text)
$K_s$	: saturated hydraulic conductivity [cm/d]
$K_r$	: $= K/K_s$ normalized hydraulic conductivity
$c$	: liquid phase concentration [μg/ml]
$S$	: solid phase concentration [μg/g soil]
$K_d$	: equilibrium sorption constant [ml/g]
$k$	: kinetic constant [1/day]
$\alpha, n, m$	: shape parameters of Van Genuchten and Mualem retention and conductivity curves
$v$	: velocity of microbial degradation [μg/ml/day]
$V_{\max}$	: maximum velocity [μg/ml/day]
$K_M$	: Michaelis constant [μg/ml]
$C_{org}$	: organic matter content
$K_{oc}$	: octanol water partition coefficient
$l$	: correlation length of a gaussian variogram function
$\Phi$	: parameter vector
$\Omega$	: sampling space of the parameter vector
$D_h$	: coefficient of hydrodynamic dispersion [cm <sup>2</sup> /s]

$\alpha_L, \alpha_T$  : longitudinal and transversal dispersivity coefficient [cm]

## Introduction

Experience with reactive transport processes at the laboratory scale i.e. in continuously stirred reactors, soil columns and lysimeters shows that, in spite of the apparent complexity of transport and degradation processes, decay curves and breakthrough curves can be described well by deterministic mathematical models in the form of differential equations. However, physical properties and the chemical composition of real soils are inhomogeneous. Frequently, this inhomogeneity is not simply a noise, which can be dealt with by averaging, but it is essential for the transport properties of a given soil. Consider water flow through a medium with a large range of water conductivities. If conductivities are spatially correlated, it is highly probable that interconnected regions of low and high conductivities occur. These are giving rise to a random flow pattern with preferential flow zones. Deterministic models function well in the laboratory under homogeneous conditions. However, homogeneous conditions do not prevail in the field. Upscaling is hence necessarily connected with the spatial variability of model parameters such as the hydraulic conductivity or the shape parameters of the water retention curve. Model parameters are therefore treated as multivariate random variates. In this paper, stochastic models of various degrees of

complexity (ranging from simple distribution functions to random field models) are incorporated in deterministic process models thus allowing the extrapolation of local fine-scale models across heterogeneous areas.

## Short Review of Model Equations

Water transport is modelled by the Richards-equation

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot \vec{q} + Q$$

$$\vec{q} = K(\theta) \nabla \psi$$

which is specified by the water retention curve and the hydraulic conductivity curve. The conductivity function is written in the form  $K = K_s K_r$ , where  $K_s$  denotes the saturated conductivity (which is a parameter) and  $K_r$  describes the functional relationship.  $K_r$  is referred to as normalized hydraulic conductivity. The normalized water content is defined by

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

Several parametrizations of empirical relationships are in use. The retention and conductivity curves according to van Genuchten (1980) and Mualem (1976), which are widely used, are flexible, i.e. they can be applied to many soil types. Where  $m = 1 - 1/n$ . The conductivity curves are parameterized as a function of the water content

$$\frac{K}{K_s} := K_r = \Theta^{\frac{1}{2}} (1 - (1 - \Theta^{\frac{1}{n}})^2)$$

or as a function of the matric potential.

$$K_r = \frac{(1 - (\alpha\psi)^{n-1} (1 + (\alpha\psi)^n)^{-m})^2}{(1 + (\alpha\psi)^n)^{\frac{2}{n}}}$$

Potential and actual evaporation are calculated by the Penman-Monteith equation and by the approach of Feddes (1978) respectively (cf. also Dieckrüger and Arning 1995).

Transport and reaction is modelled by the convection dispersion equation, which is coupled to the above water transport equation

$$\frac{\partial}{\partial t} (\theta c + \rho S) = \nabla \cdot [\theta D_h \nabla c - \vec{q} c] = kc$$

In this equation, a linear decay law is assumed, which applies well to the examples considered below. It should be kept in mind, however, that many xenobiotics such as pesticides are degraded by microbial processes with non-linear degradation kinetics such as

$$v = \frac{V_{\max} c}{c + K_M}$$

In the case of linear equilibrium binding, the solid phase concentration  $S$  is related to the liquid concentration  $c$  via

$$S = K_d c$$

where  $K_d$  is the equilibrium sorption constant. All model parameters are strongly related to soil properties, e.g. the maximum degradation rate and the strength of adsorption of many chemicals depend on the organic matter content of soil. The above equations together with appropriate boundary values and initial conditions constitute a boundary value problem.

## Concept of Random Soil Columns

The concept of random soil columns is based on the notion of an ensemble (in the statistical sense) of uncorrelated soil columns. This means that lateral flow is neglected. For each soil column, a deterministic model is valid. The statistical model consists of the probability density function of the parameter vector, which is conceived as random. Given this function, it is possible to compute the expectation and other statistical moments of the solution of the initial boundary value problem. Extrapolation from local homogeneous scale to large heterogeneous areas is carried out via the expectation operation. The solution of the initial boundary value problem, which depends on the stochastic parameters, simply acts as a transformation of probability density functions. In other words, the random parameter vector is mapped via the deterministic model into a random scalar concentration field  $c(x, t)$ .

$$\begin{pmatrix} \theta_s \\ \theta_r \\ K_s \\ \alpha \\ n \\ \rho \end{pmatrix} \rightarrow \text{boundary value problem } c(\vec{x}, t)$$

The mathematical problem involves the derivation of the density function  $f^c(c)$  from the probability density function  $f^\phi(\phi)$  of the parameter  $\phi$ . In the one-dimensional case, the density transformation is achieved via

$$f^c(c) = \frac{d}{dc} g^{-1}(c) f^\phi(g^{-1}(c))$$

with  $c = g(\phi)$ . Gustavson and Holden (1990) solved this problem for a mono-exponential decay with a Gamma distributed decay rate.

In the general case the problem is stated as follows:  
Given:

- i) a deterministic dynamical model in form of a boundary value problem with parameter vector  $\Phi$
- ii) the density function of the parameter vector  $\Phi$ ,  $f(\Phi)$

the mathematical problem is then to find estimators for the moments of the distribution of the state variables of the dynamical model.

**Table 1.** Statistical distributions of the parameters used in the Latin Hypercube simulations. Notations: *n* = normal distribution, *l* = lognormal distribution, *o* = upper soil layer, *u* = lower soil layer

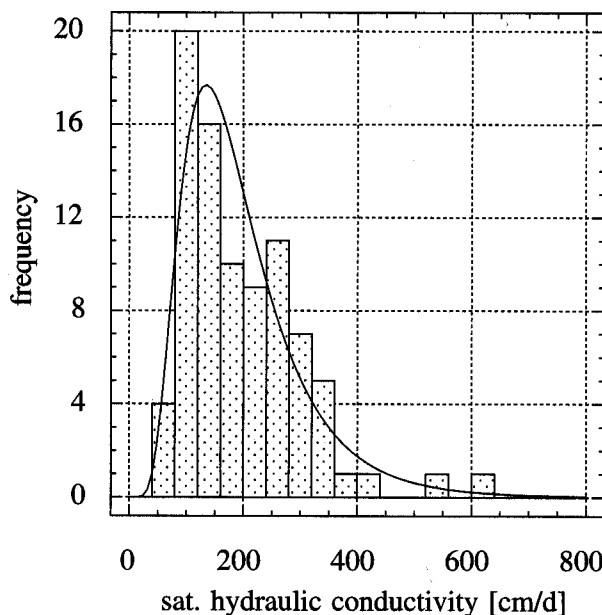
Parameter	$\mu_o$	$\sigma_o$	$\mu_u$	$\sigma_u$
$\theta_s$ (n)	0.371607	0.027761	0.299843	0.031529
$\theta_r$ (n)	0.041713	0.023728	0.024300	0.013460
$K_s$ (l)	197.9930	107.1420	260.1290	218.1420
$\alpha$ (l)	0.035921	0.015304	0.052566	0.032650
$n-1$ (l)	0.409752	0.141652	0.587983	0.325315
$\rho$ (n)	1.526470	0.087350	1.517870	0.091856
$C_{org}$ (n)	1.081160	0.193570	0.316326	0.158269

When no analytical solutions are obtainable, which is the case in nearly all practical applications, this problem is addressed by stochastic simulation methods referred to as **Stratified random sampling** and **Latin Hypercube sampling**. An intuitively appealing method is to generate a random sample of the parameter vector and to derive estimators from the sampling statistics of the model output. This approach is referred to as the Monte Carlo method. In many practical situations, the number of replications is limited by the running time of the numerical code. Therefore, sampling techniques have been developed, which are more efficient than simple random sampling (McKay *et al.*, 1979). These are stratified random sampling and Latin Hypercube sampling. Let  $\Omega$  denote the sampling space of the parameter vector  $\Phi$ . Stratified sampling is performed by partitioning  $\Omega$  into disjoint subsets and obtaining random samples from each subset. Latin Hypercube sampling is an extension of stratified sampling.

The following example is based on a soil survey based on 86 sample points. From each sample, the parameters for the water transport model were determined in two soil layers. As an example, Fig. 1 shows the histogram of the saturated hydraulic water conductivity, which can be modelled well by a lognormal distribution, as is frequently the case. Other parameters such as the saturated water content rather follow a normal density function (*cf.* Fig. 2). Table 1 summarises the type of distribution and their parameters. Since the sample points are georeferenced, geostatistical analyses could be performed and maps were generated by kriging. Fig. 3 shows the map of the silt plus clay content. This data base was used for the simulation of the transport of a tracer, bromide, and of the transport, sorption and degradation of the herbicide chlorotoluron. The  $K_d$  value of chlorotoluron was computed via the relation  $K_d = K_{oc} C_{org}$ . Although the kinetic constant  $k$  was kept fixed, the effective kinetic constant rate  $k_{eff}$  is random, since it is related to the  $K_d$  value which is in turn related to the random soil property  $C_{org}$ .

$$k_{eff} = \frac{k}{1 + \frac{\rho}{\theta} K_d}$$

Simulations were performed for the time period from 28 March 1994 to 15 October 1994 using precipitation and temperature data from the meteorological station. Initial herbicide and bromide loads were 5kg/ha. Simulations were performed a) for each of the 86 sampling points and b) for 100 Latin Hypercube realisations based on distributions and parameters as given in Table 1. Appropriate criteria are the total residues of chlorotoluron and the depth of the peak of the soil profiles of bromide at the end of the study. Figures 4 and 5 show the distribution of these measures for the two types of simulations performed. The histograms of both simulations (sample points and Latin Hypercube sampling) are similar. Furthermore, the histograms are skewed and exhibit a large range due to the spatial variability. Note that chlorotoluron residues lie in the range from 0.01 to 1.2 kg/ha for the Latin Hypercube histogram. For the simulations based on the sample points,



**Fig. 1.** Histogram of the saturated hydraulic water conductivity, upper soil layer. Note that the form of the histogram is well matched by a lognormal density function.

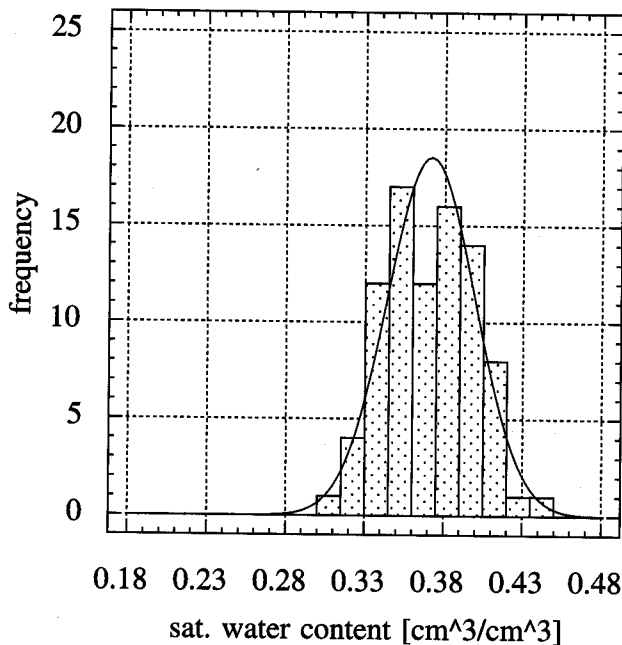


Fig. 2. Histogram of the saturated water content, upper soil layer. The form of this histogram is best described by a normal density function.

contour maps can be constructed (interpolation by kriging) as is shown in Fig. 6 and Fig. 7.

Note that the spatial aspects of these simulations are solely due to the georeferenced sampling points of the soil properties. The concept of uncorrelated soil columns without lateral flow is still valid. From the point of view of mathematics, the contour maps are the results of the transformation of a random vector, the parameter vector of the model. This random vector is assumed to be generated by a random spatial process with spatial correlations. The transformation is achieved by solving an initial boundary value problem for each sampling point. The random para-

meter vector is thus transformed into the variables 'total chlortoluron residues' and 'depth of bromide peak'. This example is continued in section 5.

## Three Dimensional Transport Processes over Realisations of Random Fields

### WATER TRANSPORT

The concept of uncorrelated soil columns is based on the assumption that lateral flow can be neglected. This assumption is valid if the soil properties are homogeneous within a soil column. If the soil consists of different layers, this assumption is made for each layer. Each soil column is then described by a one-dimensional transport model. But what if microscale variation creates a heterogeneous soil structure within a column? Parameter fields can be modelled as realisations of spatially correlated random processes. Consider for instance the hydraulic conductivity. If this parameter is the realisation of a second order stationary stochastic process with a Gaussian shape variogram, a realisation creates connected zones of different conductivities. If the correlation length is in the order of magnitude of the column under study then it is most likely that connected regions of high conductivity exist. In these regions, water flow and hence transport are facilitated. Obviously one-dimensional models are not capable of simulating these effects. How can one handle this kind of heterogeneity? A possible procedure involves the following steps:

1. Identification of the spatial random process and its parameters, e.g. the correlation length.
2. Generation of realisations of the process.
3. Three dimensional simulation of water and matter transport over realisations of the random parameter field.
4. Assessment of the statistical properties from a large number of realisations.

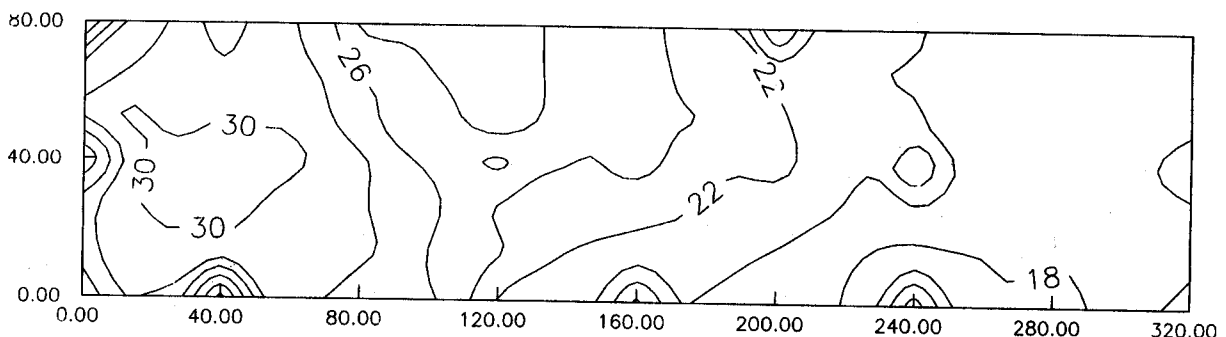


Fig. 3. Contour map of silt and clay content [% by weight] of the investigation site (coordinates in m).

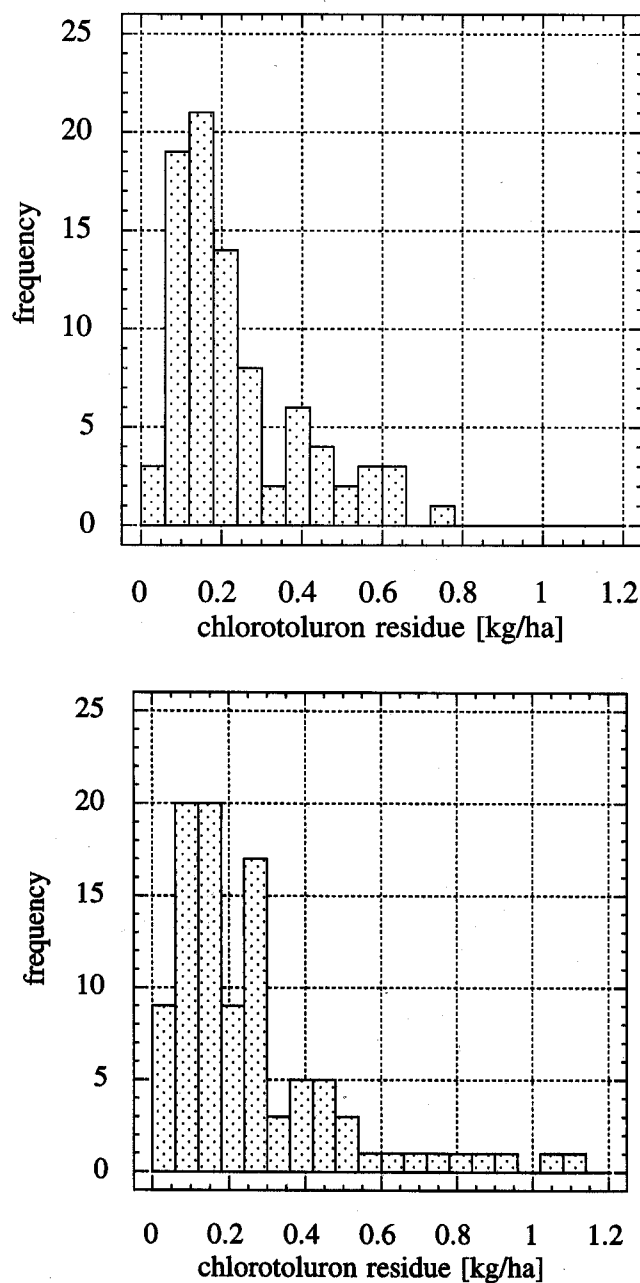


Fig. 4. Histogram of the criterion measure 'total chlorotoluron residues' a) based on the parameters as measured at the 86 sample points b) based on Latin hypercube sampling from statistical distributions (cf. Table 1).

It is assumed that the basic stochastic process is given by

$$\phi(\vec{x}) = \mu y + \omega(\vec{x}) + \epsilon$$

where  $\mu$  denotes the general mean,  $\omega$  a second order stationary process and  $\epsilon$  a white noise (uncorrelated random variable). Stationarity ensures that

$$E[\phi(\vec{x})] = \frac{1}{G} \int_G \phi(\vec{x}) d^3x = \mu y = \text{const}$$

The properties of the second order process are determined by the form of the variogram. To solve deterministic transport processes over a random field, it is necessary that the random field can be differentiated, i.e. that a smooth surface of the parameter field is generated without spikes. Fig. 8 shows such a 'smooth' parameter field. This property is

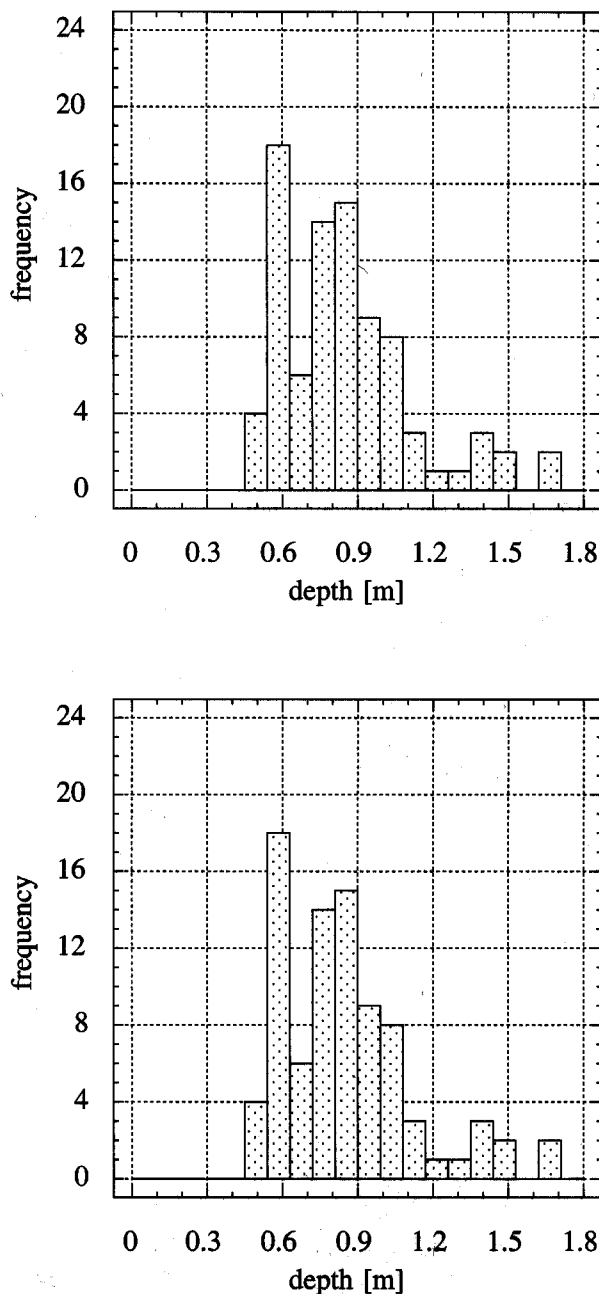


Fig. 5. Histogram of the criterion measure 'depth of bromide peak' a) based on the parameters as measured at the 86 sample points b) based on Latin hypercube sampling from statistical distributions (cf. Table 1).

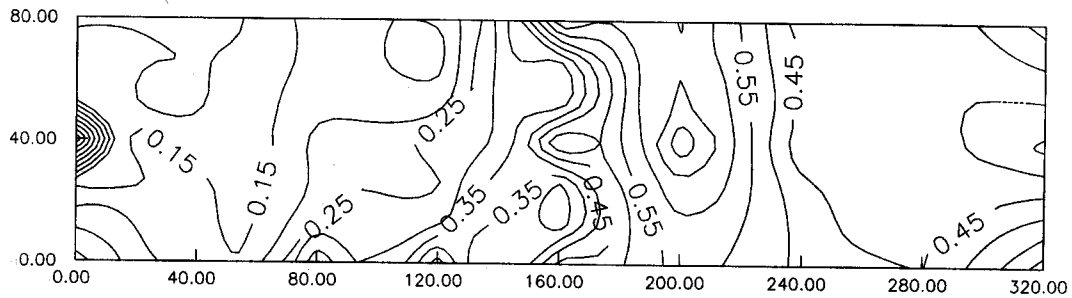


Fig. 6. Contour map of total residues of chlorotoluron based on simulations with sampled parameters.

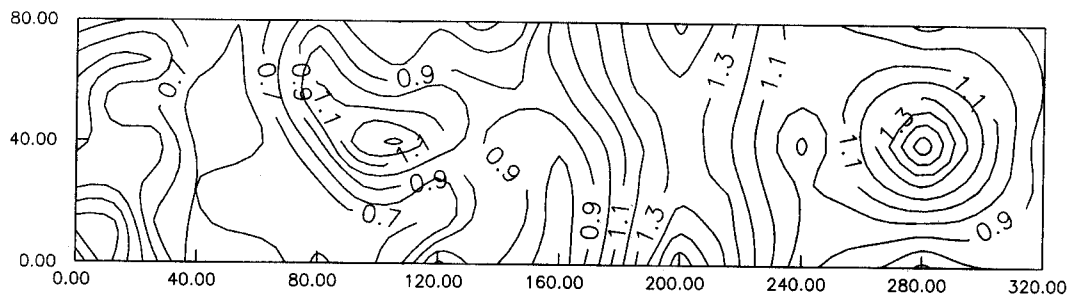


Fig. 7. Contour map of the depth of bromide peak based on simulations with sampled parameters.

ensured if the slope of the variogram in the origin is zero as is the case for the Gaussian model.

$$\gamma(\vec{h}) = \sigma^2(1 - e^{-\frac{1}{2l}|\vec{h}|^2}) \quad \vec{h} = \vec{x}_i - \vec{x}_j$$

The parameter  $l$  characterizes the correlation length.

The following example is taken from a publication by Tietje and Richter (1992). Assuming a lognormal distribution of the saturated hydraulic conductivity, the authors simulated random parameter fields and solved the Richards-equation for the stationary case in three dimensions over the realisation of random  $K_S$ -fields. Figure 8 shows a realisation of the spatial parameter field of  $K_S$ ; Fig. 9 shows the resultant flow field, which is obtained by the numerical solution of Richards-equation in three dimensions by means of the finite element method.

#### MATERIAL TRANSPORT

The application range of the one-dimensional form of the convection dispersion equation is limited to substrates with only slight spatial heterogeneities. Lateral flow becomes important if the soil contains random three-dimensional structures giving rise to random parameter fields. In a general three-dimensional situation, the coefficient of hydrodynamic dispersion  $D_h$  becomes a tensor. In a random soil, one has to generate a random tensor field. The components of the dispersion tensor depend on the components of the velocity field of the water and, in isotropic soils, on the longitudinal and transversal dispersivity coefficients  $\alpha_L$  and  $\alpha_T$ . To complicate matters, these coefficients are correlated to parameters of the water trans-

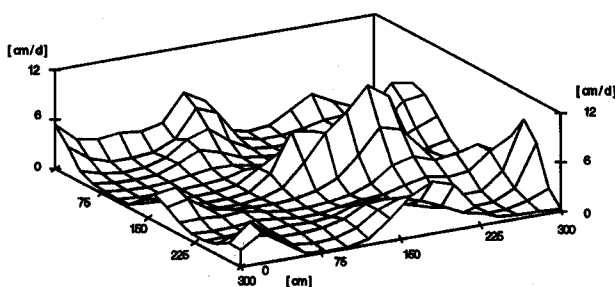


Fig. 8. Cross section through a three-dimensional realisation of a random spatial  $K_S$ -field.

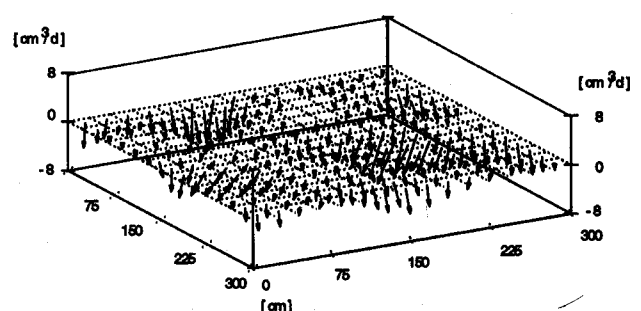


Fig. 9. Flow field over the realisation of the random spatial  $K_S$ -field shown in Fig. 8.

port. The anisotropy is due to the flow field of the water. This tensor has the general form (Bear, 1979):

$$D_{ij} = a_{ijkm} \frac{v_k v_m}{\bar{v}} f(Pe, \delta)$$

$f$  is a correction factor, which depends on the peclet number  $Pe$  and on the pore geometry.

$$Pe = \text{Peclet number} = \frac{L\bar{v}}{D_d}$$

with  $L$  being some characteristic length of the pores and  $D_d$  being the coefficient of molecular diffusion of the solute in the considered liquid phase. In most applications,  $f$  is set equal to 1. The coefficient  $a_{ijkm}$  is the element of a fourth rank tensor, the dispersivity tensor. In the isotropic case, it reduces to

$$a_{ijkm} = \alpha_T \delta_{ij} \delta_{km} + \frac{\alpha_L - \alpha_T}{2} (\delta_{ik} \delta_{jm} + \delta_{im} \delta_{jk})$$

where  $\delta_{ij}$  denotes the Kronecker symbol and  $\alpha_L$  and  $\alpha_T$  are the longitudinal and transversal dispersivity. The elements of the tensor of hydrodynamic dispersion are thus given by

$$D_{ij} = \alpha_T \bar{v} \delta_{ij} + (\alpha_L - \alpha_T) \frac{v_i v_j}{\bar{v}}$$

where  $v_j$  are the components of the water velocity field. In the following example which is taken from the PhD-thesis of A. Stock (1994), it is assumed that both coefficients are inversely proportional to the square of the hydraulic conductivity:

$$\alpha_L \propto \frac{1}{K_S^2}$$

Thus, regions of high conductivity are assumed to exhibit low dispersivity and vice versa.

In the study of Stock, stationary flow and water content fields were generated by solving the water transport equation over a random field of  $K_S$  values. In addition, a random field of the dispersivity coefficients was generated under the above assumption of an inverse proportional relationship between these coefficients and  $K_S$ . Figures 10a-c show the development in time of vertical cross sections of the three-dimensional concentration field of a slowly degradable substance. Each Figure also shows the mean concentration profile and the profile obtained from a hypothetical borehole in the centre of the region. Note the difference between the mean profile and the profile obtained from the borehole. For degradable substances, a decrease of the degradation rate with depth has to be taken into account. This effect is due to the decreasing organic matter content, which is closely related to the degradation capacity and to the decreasing oxygen content of the soil. The experience gathered from a large series of simulations stresses the importance of soil heterogeneity in two respects:

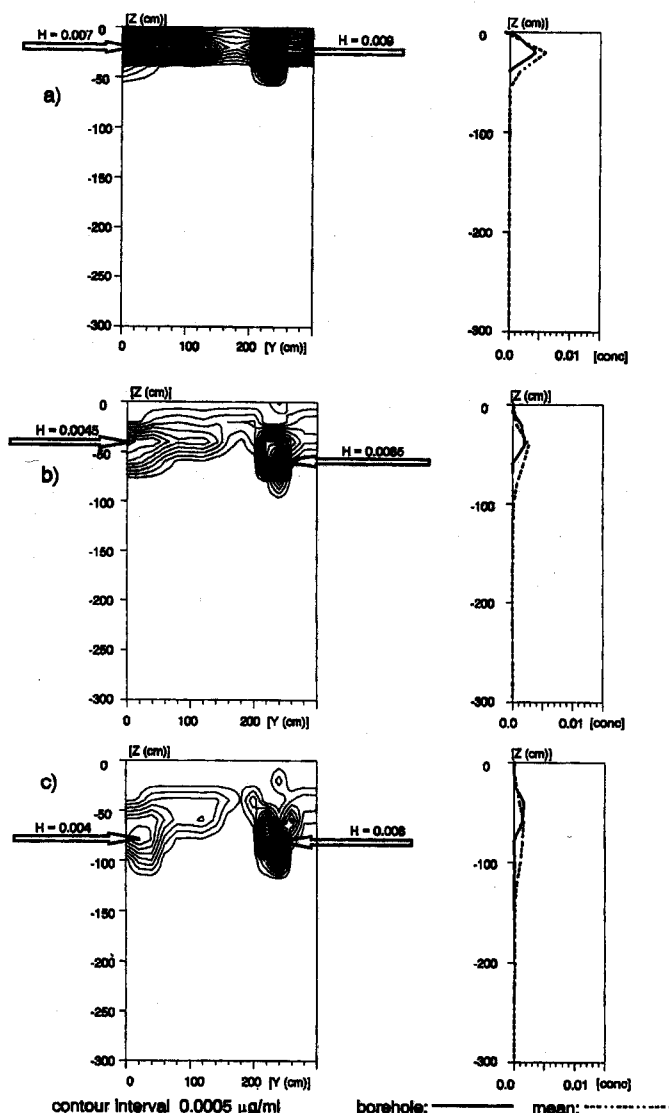


Fig. 10. Time development of a cross section of a concentration field of a slowly degradable substance in a soil with a low degree of heterogeneity. On the right side the mean depth profiles and the profiles obtained by a fictitious borehole in the middle of the cross section: a) 5 days, b) 10 days and c) 20 days after simulation start. H marks the location where the highest values occur.

The transfer to field conditions of experimental and/or simulation results obtained from artificial, homogeneous soil columns in the laboratory may lead to an underestimation of the amount of pesticide leached.

In heterogeneous soils, the information obtained from borehole profiles should be interpreted with caution. For more information see Richter *et al.* (1996) and Stock (1994).



## SOME TECHNICAL REMARKS

The one-dimensional partial differential equations were solved by a fully implicit finite difference scheme. The realisations of the spatial random fields were generated by the turning bands method (Mantoglou and Wilson 1982). The underlying variograms are Gaussian. Variogram models with zero slope at the origin generate sufficiently smooth (differentiable in the stochastic sense) random fields, which is necessary to ensure the existence of the solution of the initial boundary value problem. The three-dimensional initial boundary value problem was solved by the method of finite elements.

## Representative Parameter Sets and Parameter Fields

## RANDOM SOIL COLUMNS

The concept of random soil columns is applicable only if lateral flow can be neglected. This implies that the correlation lengths of the underlying spatial fields are large so that microscale patterns influence the flow field only weakly. First, the case of a known density function is considered. This demands that the sample size is very large so the distribution law can be identified. Since the state variables of the deterministic models are spatio-temporal concentration fields, one has to define criteria such as the total amount of residues in a soil layer or the depth of the peak of the concentration profile at a prescribed time point. The recommended procedure is then straightforward:

aggregation of the spatio-temporal concentration field generated by the deterministic model by an appropriate measure, e.g. the total residual mass of a pesticide in the upper soil layer.

calculation of measures either by direct integration or by the Latin Hypercube method.

construction of histograms and percentile bands for the measures. This can be done either by density transformation techniques or by the Latin Hypercube method (McKay *et al.* 1979). The latter method has a larger range of application. The former demands a density transformation.

selection of a parameter set, which results in a criterion of the modal class as **representative parameter set**.

Extrapolation to large areas is then based on the representative set.

Unfortunately, sample sizes in practice are generally very small and the type of density function cannot be identified, or the data do not match any classical model such as a normal or lognormal density function. In this case, Latin Hypercube methods still apply. Calculations can be performed on the basis of the empirical distribution functions or histograms. In large scale applications, model parameters have to be derived from the information contained in soil survey maps. The derivation of model parameters from this kind of information is achieved via so-called pedo-transfer functions (Tietje and Tapkenhinrichs 1993).

Summarising the example of the last section, the histograms of the target variables 'total chlorotoluron residues' and 'bromide peak depth' are shown in Figs. 4 and 5. Table 2 summarises the statistical parameters of the histograms. The table also contains the results of a simulation performed with the means of the underlying parameters (cf. Table 1). They are close to the values obtained by averaging the results of single simulations.

Table 3 summarises the representative parameters for the two soil layers. It was possible to find parameter sets, which yield values in the modal class of both criterion measures.

## HIGHLY SPATIALLY CORRELATED PARAMETER FIELDS

In soils with highly correlated parameter fields, heterogeneous patterns emerge within the spatial dimension of a soil column. Only three-dimensional models are capable of simulating water and matter flow in such environments. One has to recall that an effective parameter is meant to replace an inhomogeneous block of soil by an equivalent homogeneous one. It is obvious that this approach yields only crude approximations in a block of soil with complicated spatial patterns, especially if degradation is involved. Hence, in this situation, effective parameters are of only limited value and a new concept based on the notion of a **representative parameter field** is proposed.

1. Aggregation of the spatio-temporal concentration field generated by the deterministic model by an appropriate

**Table 2.** Mean values and standard deviations of the criterion measures 'total chlorotoluron residues' and 'depth of bromide peak'. The last column shows the results obtained by a simulation based on the expectation of the model parameters. Note the close agreement with the values obtained by averaging the simulation results. Notations: *LH* = Latin Hypercube, *S* = Simulation of sample points, *M* = mean parameter values

Criterion measure	$\mu_S$	$\sigma_S$	$\mu_{LH}$	$\sigma_{LH}$	$\mu_M$
total residues CT [kg/ha]	0.237	0.163	0.260	0.222	0.236
depth of bromide peak [m]	0.855	0.265	0.843	0.224	0.875

**Table 3.** Representative parameters derived from the modal classes of the histograms of the criterion measures 'total chlorotoluron residues' and 'depth of bromide peak'. Note that the parameters chosen result in values of the modal classes of both criterion measures. Notations: *LH* = Latin Hypercube, *S* = Simulation of sample points, *u* = upper layer, *l* = lower layer.

	$\theta_s$	$\theta_r$	$K_s$	$\alpha$	$\rho$		$C_{org}$
LH u	0.37	0.037	312	0.046	1.50	1.49	0.98
S u	0.33	0.0	120	0.038	1.20	1.58	0.95
LH l	0.38	0.055	308	0.098	1.70	1.61	0.36
LH l	0.28	0.0	132	0.057	1.251	1.73	0.33

**Table 4.** Model approaches at different scales

Scale	Stochastic properties of model parameters	Model
continuously stirred tank reactor	uncertainties due to experimental error	kinetic models in form of ordinary differential equations
artificial column reactor	almost homogeneous microscale variation uncertainties due to experimental error	kinetic models coupled with <b>one-dimensional</b> transport models in form of partial differential equations plus multivariate statistical distribution functions of the parameter-vector distribution functions pertain to <b>one soil column</b>
field scale (low spatial correlation) one pedological unit	(statistical ) ensemble of soil columns	kinetic models coupled with <b>one-dimensional</b> transport models in form of partial differential equations plus multivariate statistical distribution functions of the parameter-vector distribution functions pertain to the soil properties of a field
field scale (high spatial correlation) one pedological unit	soil properties realisations of a three-dimensional random spatial process	kinetic models coupled with <b>three-dimensional</b> transport models in form of partial differential equations plus three-dimensional multivariate random field models for soil properties
catchment scale collection of pedological units (low spatial correlation)	several statistical ensembles of soil columns	kinetic models coupled with <b>one-dimensional</b> transport models ... plus distribution functions of soil parameters for each pedotope
catchment scale collection of pedological units (high spatial correlation)	soil properties realisations of a collection of three-dimensional random spatial processes	kinetic models coupled with <b>three-dimensional</b> transport models ... plus random field models for each pedotope

measure, e.g. the total residual mass of a pesticide above the plough horizon.

2. Production of realisations of the spatial random process.
3. Calculation of the criterion value for each realisation.
4. Construction of percentile bands and the histogram of the criterion.
5. Consideration of the realisations which belongs to the modal value of the histogram as the representative parameter field.

#### DIFFERENT SOIL TYPES

The concept of a random spatial parameter field can be extended to regions of different soil types. The soil type determines the parameters of the continuous spatial random process. The distribution of soil types can be modelled by stochastic geometries (so called boolean models) and in a second step, for each soil type a continuous random field is generated.

## Conclusions

The translation of environmental fate models across scales necessitates the combination of deterministic approaches in the form of systems of partial differential equations with stochastic models. Table 4 summarises the proposed model approaches and combinations of deterministic and stochastic models at different scales in dependence of the stochastic properties of the underlying soil parameters.

The key idea of this paper is that the statistical methods in use for an ensemble of random soil columns can be extended to spatial random process models by introducing a representative parameter field. The proposed procedure involves the steps

1. Construction of random field models
2. Solving initial boundary value problems over realisations of random parameter fields
3. Selection of a representative field

In this context, a pedological unit is characterized by a random field model. The pedological units in turn are combined to catchments and landscapes. Whereas this concept for translating models across scales is quite appealing from a theoretical point of view, how to identify the many spatial random processes involved, is by no means clear. It is hoped that it will be feasible to associate a

proper random field model to each pedotope taking into account both the properties of a soil and its genesis.

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